

# Quantum Algorithm for Solving an NP-Complete Problem

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When a probe qubit is coupled to a quantum register that represents a physical system, the probe qubit will exhibit a dynamical response only when it is resonant with a transition in the system. Using this principle, we propose a quantum algorithm for solving a specific NP-complete problem, the 3-bit Exact Cover problem, EC3. We show that on a quantum computer, the number of qubits increases linearly with the size of the EC3 problem, while the efficiency of the algorithm is independent of the size of the problem. Our results indicate that quantum computers may be able to outperform classical computers in solving NP-complete problems.

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Extraordinary progress has been made in the field of quantum computation since the discovery of Shor's factoring algorithm [1] and Grover's search algorithm [2]. It was found that quantum computing offers speedup for a number of problems [3, 4]. Classically, problems can be divided into two groups, those that can be solved in polynomial time (P) and the nondeterministic polynomial (NP) problems for which no polynomial-time algorithms are known. NP-complete (NPC) problems are a subclass of NP problems. Solving one NPC problem in polynomial time means that all NPC problems can be solved in polynomial time. The question of whether there are polynomial-time algorithms for NPC problems is an unsolved problem in mathematics [5, 6]. It is also not known whether or not NPC problems can be solved in polynomial time on quantum computers. In this paper, using the principle that when a probe qubit is coupled to a quantum register that represents a physical system the probe qubit will exhibit a dynamical response only when it is resonant with a transition in the system, we propose a polynomial-time quantum algorithm for solving a specific NPC problem, the 3-bit Exact Cover problem, EC3.

The EC3 problem is a restricted version of the 3-bit satisfiability (3-SAT) problem [7]. No algorithm has been found that can solve this problem in polynomial time. In Ref. [7, 8], Farhi and coworkers developed a quantum adiabatic algorithm (QAA) for solving the EC3 problem. In the QAA for solving the EC3 problem, one starts from an initial Hamiltonian,  $H_B$ , and its ground state as the initial state, and evolves  $H_B$  to a final Hamiltonian  $H_P$ , whose ground state is the solution to the EC3 problem. The system is evolved from the initial state to the ground state of  $H_P$ . The computation time  $t$  increases as  $t \sim g_{\min}^{-2}$ , where  $g_{\min}$  is the minimum energy gap between the ground and the first excited state during the evolution. The cost of the QAA is determined by the scaling of  $g_{\min}$  with the size of the EC3 problem (here, the size of the EC3 problem is defined as the number of bits in the problem). It has been found that the QAA cannot solve the 3-SAT problem, or the EC3 problem, efficiently [9–13]. Here by applying a quantum algorithm we developed

recently [14], we present a quantum algorithm for solving the EC3 problem.

The EC3 problem on a quantum computer can be formulated as follows [7, 8]: the 3-bit instance of satisfiability is a Boolean formula with  $M$  clauses

$$C_1 \wedge C_2 \wedge \cdots \wedge C_M, \quad (1)$$

where each clause  $C_l$  is true or false depending on the values of some subset of the  $n$  bits, and each clause contains three bits. The clause is true if and only if one of the three bits is 1 and the other two are 0. Let  $i_C$ ,  $j_C$  and  $k_C$  be the 3 bits associated with clause  $C$ . For each clause  $C$  define an “energy” function

$$h_C(z_{i_C}, z_{j_C}, z_{k_C}) = \begin{cases} 0, & \text{if } (z_{i_C}, z_{j_C}, z_{k_C}) \text{ satisfies clause } C \\ 1, & \text{if } (z_{i_C}, z_{j_C}, z_{k_C}) \text{ violates clause } C \end{cases} \quad (2)$$

Then

$$H_{P,C}|z_1 z_2 \cdots z_n\rangle = h_C(z_{i_C}, z_{j_C}, z_{k_C})|z_1 z_2 \cdots z_n\rangle, \quad (3)$$

where  $|z_j\rangle$  is the  $j$ -th bit and has the value 0 or 1. Define

$$H_P = \sum_C H_{P,C}. \quad (4)$$

$H_P|\psi\rangle = 0$ , if and only if  $|\psi\rangle$  is a superposition of states of the form  $|z_1 z_2 \cdots z_n\rangle$ , where the bit string  $z_1 z_2 \cdots z_n$  satisfies all of the clauses. If formula (1) has no satisfying assignments, the ground state (or states) of  $H_P$  corresponds to the assignment (or assignments) that violates the smallest number of clauses. The computational basis of  $|z_1 z_2 \cdots z_n\rangle$  is of dimension  $N = 2^n$ . The task is to find out if there is one (or more) of the  $2^n$  assignments that satisfies all of the clauses, that is, makes formula (1) true.

In the previous work [14], we proposed a quantum algorithm for obtaining the energy spectrum of a physical system. In this algorithm, we couple the system to a probe qubit with a certain frequency, set the probe qubit in its excited state, evolve the whole system for some time, then perform a measurement on the probe qubit.

When the frequency of the probe qubit matches the transition frequency between two energy levels of the system, one observes a peak in the decay rate of the probe qubit. Therefore by varying the frequency of the probe qubit, we can locate the transition frequencies of the system. With a little variation, this algorithm can also be used for solving the EC3 problem. The details are shown below.

We construct a Hamiltonian  $\tilde{H}$  that has the form:

$$\tilde{H} = \begin{pmatrix} -I_N & 0 \\ 0 & H_P \end{pmatrix}, \quad (5)$$

where  $I_N$  is the  $N$ -dimensional identity operator, and  $\tilde{H}$  acts on the state space of a  $(n+1)$ -qubit quantum register  $R_S$ . We let a probe qubit couple to  $R_S$ , and design a Hamiltonian  $H$  for the whole system of the form

$$H = \frac{1}{2}\omega\sigma_z + \tilde{H} + c\sigma_x \otimes A, \quad (6)$$

where the first term is the Hamiltonian of the probe qubit, the second term is the Hamiltonian for the quantum register  $R_S$ , and the third term describes the interaction between the probe qubit and  $R_S$ . Here,  $\omega$  is the frequency of the probe qubit (we have set  $\hbar = 1$ ), and  $c$  is the coupling strength between the probe qubit and  $R_S$ , while  $\sigma_x$  and  $\sigma_z$  are Pauli matrices. The operator  $A$  acts on the state space of  $\tilde{H}$  and plays the role of an excitation operator. It contains all possible excitation operators that excites the states from subspace of  $-I_N$  to subspace of  $H_P$ ,

$$A = \frac{1}{\sqrt{N}}(A_1 + A_2 + \cdots + A_N), \quad (7)$$

where  $A_1 = \sigma_x \otimes I_2 \otimes I_2 \otimes \cdots \otimes I_2$ ,  $A_2 = \sigma_x \otimes I_2 \otimes \cdots \otimes I_2 \otimes \sigma_x$ ,  $\dots$ ,  $A_{n+1} = \sigma_x \otimes \sigma_x \otimes I_2 \otimes I_2 \otimes \cdots \otimes I_2$ ,  $A_{n+2} = \sigma_x \otimes I_2 \otimes \cdots \otimes I_2 \otimes \sigma_x \otimes \sigma_x$ ,  $A_{n+3} = \sigma_x \otimes I_2 \otimes \cdots \otimes \sigma_x \otimes I_2 \otimes \sigma_x$ ,  $\dots$ ,  $A_N = \sigma_x \otimes \sigma_x \otimes \cdots \otimes \sigma_x \otimes \sigma_x$ , where  $I_2$  is the two-dimensional identity operator. Even though the operator  $A$  has an exponentially large number of terms, it can be implemented at polynomial cost as

$$A = \sigma_x \otimes \left[ \frac{1}{\sqrt{2}}(I_2 + \sigma_x) \right]^{\otimes n}. \quad (8)$$

We prepare  $R_S$  in the state

$$|\Psi_s\rangle = \frac{1}{\sqrt{N}} \sum_{i=1}^N |\varphi_i\rangle = \frac{1}{\sqrt{N}} \sum_{i=1}^N |0\rangle \otimes |\chi_i\rangle, \quad (9)$$

as the reference state, where  $|\chi_i\rangle$  are the states of the computational basis in the subspace of  $I_N$ , and  $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ . This is achieved by initializing  $R_S$  in state  $|0\rangle^{\otimes(n+1)}$  and applying the operator  $I_2 \otimes H_d^{\otimes n}$ , where  $H_d$  is the Hadamard gate. The states  $|\varphi_i\rangle$  are the eigenstates of  $\tilde{H}$  with eigenvalues  $-1$  and with a degeneracy of

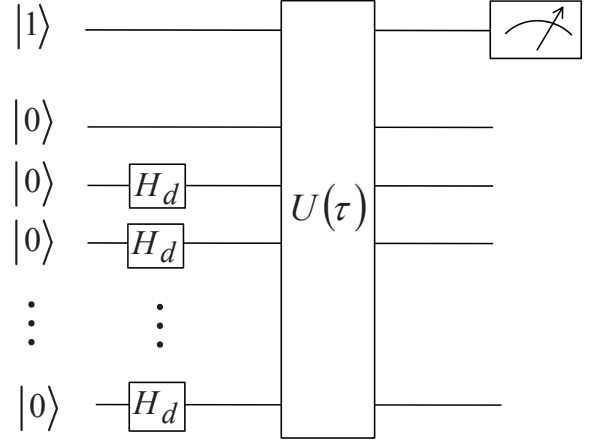


FIG. 1: Quantum circuit for solving the Exact Cover problem EC3. The first line represents a probe qubit, and the next  $n+1$  lines represents the quantum register  $R_S$ .  $H_d$  represents the Hadamard gate, and  $U(\tau)$  is the time evolution operator with Hamiltonian given in Eq. (6).

$N$ , therefore the reference state  $|\Psi_s\rangle$  has the eigenvalue  $-1$ . We set the frequency of the probe qubit  $\omega = 1$ , and run the circuit in Fig. 1. Let the whole system evolve with the Hamiltonian shown in Eq. (6) for time  $\tau$ . After that, we read out the state of the probe qubit. We repeat this procedure many times in order to obtain the decay probability of the probe qubit.

In the procedure above, setting the probe qubit frequency  $\omega = 1$ , we can probe the transition between the initial state, whose eigenvalue is  $-1$ , and the eigenstate of  $\tilde{H}$  with corresponding eigenvalue  $0$ , which encodes the solution to the EC3 problem. If there exists at least one assignment that satisfies all of the clauses, a decay of the probe qubit will be observed. The assignment is encoded in the state of the last  $n$  qubits of the quantum register  $R_S$ . If there is no assignment that satisfies all of the clauses, we can increase  $\omega$  by 1 each time and run the algorithm. Since the eigenvalues of the Hamiltonian  $H_P$  are integers, if we keep increasing the frequency of the probe qubit by 1 and run the algorithm, we will find the assignment that violates the smallest number of clauses.

The procedure of the algorithm is summarized as follows: (i) prepare a probe qubit in state  $|1\rangle$  and a  $(n+1)$ -qubit quantum register  $R_S$  in state  $|0\rangle^{\otimes(n+1)}$ ; (ii) apply operator  $I_2 \otimes H_d^{\otimes n}$  on  $R_S$ , therefore  $R_S$  is transformed into state  $|\Psi_s\rangle$  as shown in Eq. (9); (iii) implement the time evolution operator  $U(\tau) = \exp(-iH\tau)$  where  $H$  is given in Eq. (6); (iv) read out the state of the probe qubit; (v) perform steps (i) – (iv) many times in order to obtain good statistics and calculate the decay probability of the probe qubit. The quantum circuit for steps (i) – (iv) is shown in Fig. 1.

In our algorithm,  $n+2$  qubits are required for solving an  $n$ -bit EC3 problem on a quantum computer, which

increases linearly with the size of the problem. In the following, we discuss the efficiency of the algorithm.

The efficiency of the algorithm is defined as the number of times that the circuit in Fig. 1 must be run in order to obtain the decay probability,  $P_{\text{decay}}$ . The number of times that the circuit needs to be run must be at least proportional to  $1/P_{\text{decay}}$  in order to obtain  $P_{\text{decay}}$ .

As we discussed in Ref. [14], the decay probability of the probe qubit is:

$$P_{\text{decay}} = \sin^2\left(\frac{\Omega_{ij}\tau}{2}\right) \frac{Q_{ij}^2}{Q_{ij}^2 + (E_j - E_i - \omega)^2} |\langle \lambda_i | \Psi_s \rangle|^2, \quad (10)$$

where  $Q_{ij} = 2c|\langle \lambda_j | A | \lambda_i \rangle|$ , and  $\Omega_{ij} = \sqrt{Q_{ij}^2 + (E_j - E_i - \omega)^2}$ .  $|\lambda_i\rangle$  is the  $i$ -th energy eigenstate and  $E_i$  is the corresponding eigenenergy of the system, and according to Eq. (4),  $E_i$  are discrete integers. Eq. (10) describes Rabi-oscillation dynamics, where the system and probe exchange an excitation.

If a solution to the EC3 problem exists, the excitation frequency between the initial state  $|\Psi_s\rangle$  and the state with eigenvalue 0, which is the solution to the problem, is 1. With the probe qubit frequency being set to  $\omega = 1$ , and considering the degeneracy of  $|\varphi_i\rangle$ , the decay probability of the probe qubit becomes

$$P_{\text{decay}} = \sin^2\left(\frac{\Omega_0\tau}{2}\right), \quad (11)$$

where

$$\begin{aligned} \Omega_0 &= 2c|\langle \psi | A | \Psi_s \rangle| \\ &= 2c \sum_{i=1}^N \sum_{j=1}^m \frac{1}{\sqrt{Nm}} |1| \langle \mu_j | A | \varphi_i \rangle| \\ &= 2c\sqrt{m}. \end{aligned} \quad (12)$$

This term describes the summation over all excitation channels in the Rabi-oscillation. Here  $|\psi\rangle = \sum_{j=1}^m |1\rangle |\mu_j\rangle / \sqrt{m}$  encodes the solution to the EC3 problem which is a superposition of all  $m$  assignments that satisfy all of the clauses. And  $|\mu_j\rangle$  are these assignments, which are the basis states of  $H_P$  with eigenvalues 0 and have degeneracy  $m$ . From Eq. (12), we can see that as  $m$  increases, there will be more excitation channels and the period of  $P_{\text{decay}}$  will decrease. By knowing  $\Omega_0$ , we can choose a specific evolution time  $\tau$  by considering the degeneracy of the ground state of the problem, such that the probe qubit has high decay probability, therefore the algorithm has high efficiency. By trying a few times, we can find the optimal evolution time  $\tau$  for implementing the algorithm.

From the equations above, we can see that the decay probability, and therefore the efficiency of the algorithm, depends on the coupling strength  $c$  and the evolution time  $\tau$ . In general, we need to set  $c$  to be small so that

we have weak system-probe coupling and low noise. The evolution time  $\tau$  should be large, such that the change of the system is clear and one obtains high decay probability. From Eq. (11), we can see that the efficiency of the algorithm is independent of the size of the problem. Therefore by choosing appropriate  $c$  and  $\tau$ , the EC3 problem can be solved efficiently on a quantum computer using our algorithm.

When we set  $\omega = 1$ , the coupling between the initial state and all the other states except the state with eigenvalue equals to zero also contribute to the decay probability of the probe qubit, therefore introduce an error in  $P_{\text{decay}}$ . We now evaluate this error,  $P_{\text{decay}}^{\text{err}}$ .

$$\begin{aligned} P_{\text{decay}}^{\text{err}} &= \sum_{j=2}^N \sin^2\left(\frac{\Omega_{0j}\tau}{2}\right) \frac{Q_{0j}^2}{Q_{0j}^2 + (E_j - E_0 - \omega)^2} \\ &< \sum_{j=2}^N \frac{\Omega_{0j}^2}{E_j^2} \\ &\leq \sum_{j'=2}^{N_m} \frac{4c^2 m_j}{(j' - 1)^2} \\ &< 4c^2 m_0 \frac{\pi^2}{6} = \frac{2}{3} m_0 \pi^2 c^2, \end{aligned} \quad (13)$$

where  $E_0 = -1$ , is the eigenvalue of the reference state,  $m_j$  represents the degeneracy of the assignments that have eigenvalue  $E_j$ .  $N_m$  is the eigenenergy of the highest energy level of the problem, and as  $N_m \rightarrow \infty$ ,  $\sum_{j'=2}^{N_m} \frac{1}{(j'-1)^2} = \frac{\pi^2}{6}$ .  $m_0$  is the maximum of  $m_j$ . The term  $2m_0\pi^2 c^2/3$  can be small since  $c$  can be set small. Therefore we can control this error and make it very small.

In the following, we present an example that demonstrates how the algorithm would perform.

Consider an 8-bit EC3 problem, we choose three cases of the 3-bit sets of clauses, which have one, two and four satisfying assignments to the problem, respectively. As discussed above, 10 qubits are required for solving this problem using our algorithm. We set the coupling coefficient  $c = 0.002$ , and run the algorithm with different evolution time  $\tau$ . As the probe qubit decays to the state  $|0\rangle$ , the state of the last 8 qubits of the quantum register  $R_S$  encodes the solution to the above EC3 problem. Case *i*): the 3-bit sets are  $\{1, 2, 8\}$ ,  $\{2, 3, 6\}$ ,  $\{2, 3, 7\}$ ,  $\{2, 4, 5\}$ ,  $\{2, 5, 6\}$ , and  $\{3, 5, 8\}$ . The solution to the 8-bit EC3 problem for this case is  $|00010111\rangle$ . Case *ii*): the 3-bit sets are chosen to be  $\{1, 4, 5\}$ ,  $\{1, 7, 8\}$ ,  $\{2, 4, 8\}$ ,  $\{2, 7, 8\}$ ,  $\{4, 5, 8\}$ , and  $\{5, 6, 7\}$ . The solution to the problem for this case is  $|00010010\rangle$  and  $|00110010\rangle$ . Case *iii*): the 3-bit sets are  $\{1, 3, 5\}$ ,  $\{1, 6, 8\}$ ,  $\{2, 4, 6\}$ ,  $\{2, 6, 8\}$  and  $\{4, 5, 7\}$ . The solution to the problem for this case is  $|00001100\rangle$ ,  $|00100110\rangle$ ,  $|00110001\rangle$ , and  $|11000010\rangle$ .

In Fig. 2, we show the variation of simulated  $P_{\text{decay}}$  with the evolution time  $\tau$  for the above three cases. The

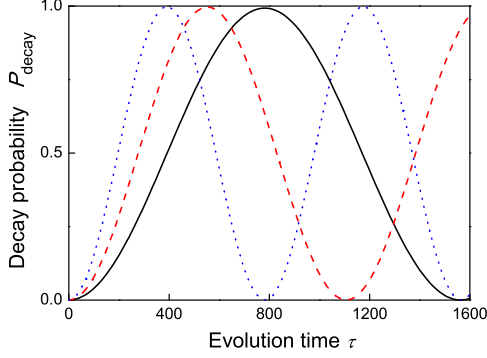


FIG. 2: Decay probability of the probe qubit vs. evolution time  $\tau$ . The frequency of the probe qubit  $\omega = 1$  and the coupling strength  $c = 0.002$ . The black solid line shows the result for case *i*): the 3-bit sets are  $\{1, 2, 8\}$ ,  $\{2, 3, 6\}$ ,  $\{2, 3, 7\}$ ,  $\{2, 4, 5\}$ ,  $\{2, 5, 6\}$ , and  $\{3, 5, 8\}$ ; the red dashed line shows the result for case *ii*): the 3-bit sets are  $\{1, 4, 5\}$ ,  $\{1, 7, 8\}$ ,  $\{2, 4, 8\}$ ,  $\{2, 7, 8\}$ ,  $\{4, 5, 8\}$ , and  $\{5, 6, 7\}$ ; and the blue dotted line shows the result for case *iii*): the 3-bit sets are  $\{1, 3, 5\}$ ,  $\{1, 6, 8\}$ ,  $\{2, 4, 6\}$ ,  $\{2, 6, 8\}$  and  $\{4, 5, 7\}$ .

black solid line, the red dashed line and the blue dotted line show the results for cases *i*), *ii*) and *iii*), respectively. In the above three cases, the decay probability almost reaches one at  $\tau = 800$ ,  $\tau = 550$  and  $\tau = 400$ , respectively. This shows that the algorithm can be run efficiently. From the figure we can also see that as the number of satisfying assignments increases, the period of  $P_{\text{decay}}$  decreases. The simulated  $P_{\text{decay}}$  fits well to the analytical results predicted by Eq. (11).

We now discuss the implementation of the algorithm. In the algorithm, we have to implement the time evolution operator  $U(\tau) = \exp(-iH\tau)$ . In the Hamiltonian  $H$ , the first two terms commute, while they do not commute with the third term. As shown in Eq. (8), the third term can be implemented efficiently using only  $(n + 2)$  gates. The operator  $U(\tau)$  can be implemented using the procedure of quantum simulation based on the Trotter-Suzuki formula [15]:

$$U(\tau) = \left[ e^{-i(\frac{1}{2}\omega\sigma_z + \tilde{H})\tau/L} e^{-i(c\sigma_x \otimes A)\tau/L} \right]^L + O\left(\frac{1}{L}\right), \quad (14)$$

where  $L$  does not depend on the size and the Hamiltonian of the problem, it can always be chosen sufficiently large such that the error is bounded by some threshold [16]. The second term of the Hamiltonian  $H$ ,  $\tilde{H}$ , as shown in Eq. (5), can be seen as a Controlled- $H_P$  ( $C-H_P$ ) operation. The operation that calculates  $H_P$  can be taken as an oracle. In our algorithm, this oracle is entangled with the probe qubit. The number of times that the  $C-H_P$  oracle is implemented is  $L$ . Therefore the implementation of  $U(\tau)$  scales polynomially with the size of the problem.

In our algorithm for solving the EC3 problem, we con-

struct a Hamiltonian that contains the Hamiltonian of the problem and a Hamiltonian with the same dimension  $N$  of the problem, whose eigenstates have degeneracy  $N$  and eigenvalues (in our case,  $-1$ ) lower than the smallest eigenvalue of the problem, and are used as a reference point. If a solution to the problem exists, we will observe the decay of the probe qubit at the excitation frequency (in our case, 1) between the reference state and the eigenstates with eigenvalue zero. In this case the system register evolves to its ground state, which is a superposition state of the assignments to the problem. If there is no solution to the problem, we can increase the frequency of the probe qubit discretely (since the energy function of the problem is discrete), and record the decay probabilities of the probe qubit. The first frequency at which the decay of the probe qubit indicates the ground state of the system, which is the solution that violates the smallest number of clauses. This algorithm can also be used for efficiently solving some other discrete mathematical problems, such as some combinatorial optimization problems.

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